

N THE CLAIMS

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11. (Amended) A computer for determining at least a portion of the structure coordinates corresponding to X-ray diffraction data obtained from a molecule or molecular complex, wherein said computer comprises:

- a) a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said data comprises at least a portion of the structural coordinates of the JNK3 complex according to Figure 1;
- b) a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said data comprises X-ray diffraction data obtained from said molecule or molecular complex;
- c) a working memory for storing instructions for processing said machine-readable data of (a) and (b);
- d) a central-processing unit coupled to said working memory and to said machine-readable data storage medium of (a) and (b) for performing a Fourier transform of the machine readable data of (a) and for processing said machine readable data of (b) into structure coordinates; and
- e) a display coupled to said central-processing unit for displaying said structure coordinates of said molecule or molecular complex.
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